NASA SBIR/STTR Technologies

MULTI-SCALE, MULTI-PHYSICS SOFTWARE FOR DESIGN OF INTEGRATED NANOBIOSYSTEMS

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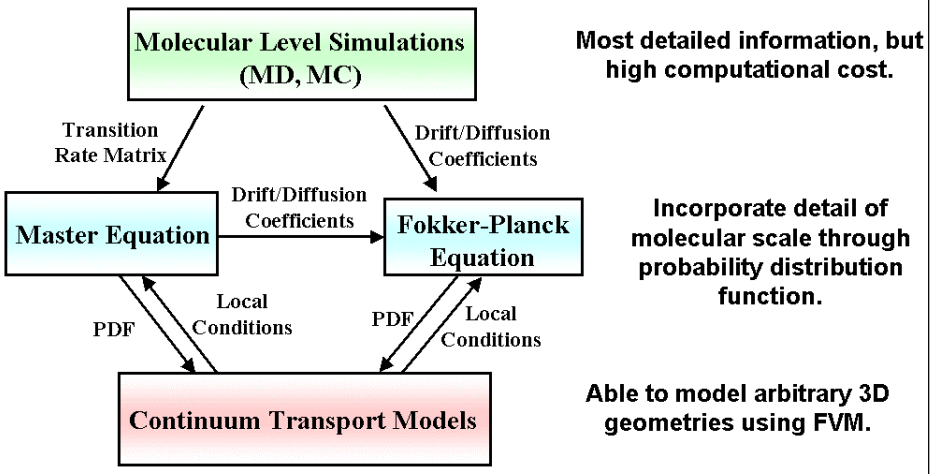
Proposal No.: B5.03-7223

Description and Objectives:

- **Current Status:** Confluence of nanotechnology and biology holds great promise to science and to society vi integrated nanobiosystems. Design of these complex products requires characterization of the nano and device scale and their interaction. Currently there are no commercial multiscale software suites supporting design of nanoscale bio-devices.
- **Objective:** Develop a universal method for coupling nanoscale physics to continuum using stochastic methods. Demonstrate capability on DNA nanopore sequencing device.



Approach:

- Generate molecular model of a DNA nanopore system.
- Perform molecular level simulations to the internal energy surface of the nanopore.
- Construct a Fokker-Planck Equation from the internal energy surfaces of the nanopore to compute the translocation rates for each DNA base, and for the chain as a whole.
- Couple the Fokker-Planck model to the convective diffusive transport equations as a source term.
- Demonstrate the value of the new tool on a nanopore seqencing device.

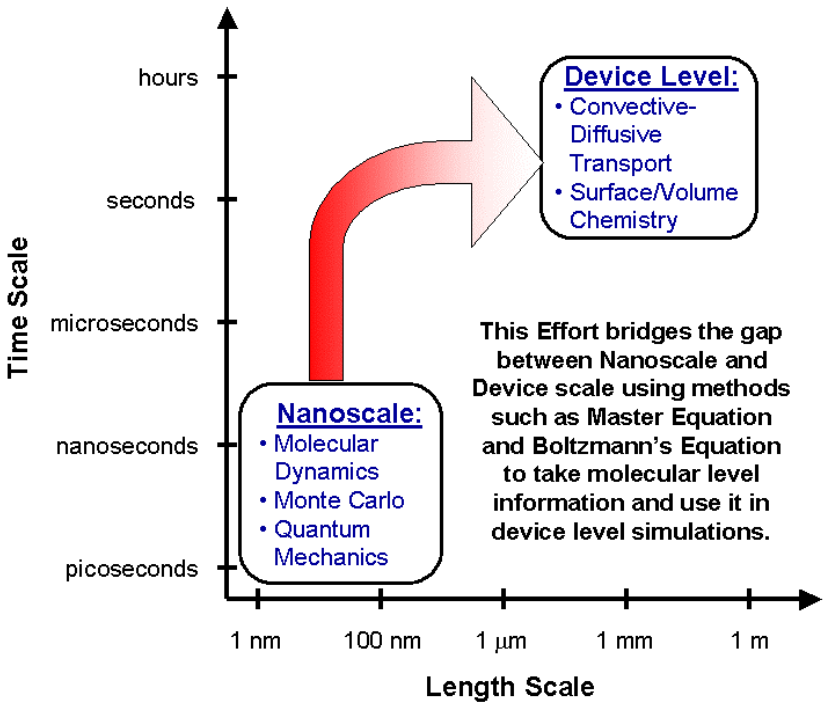
Schedule and Deliverables:

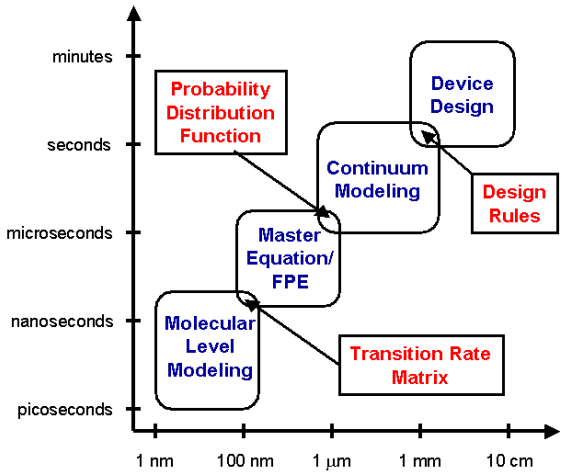
- Phase I:
  - Develop generalized methods to couple stochastic to device level.
  - Demonstrate the technique on DNA nanopore sequencer.
- Phase II:
  - Develop nanoscale unit operations general enough to handle many different types of physics.
  - Develop software further (GUI, external databases, …)

NASA & Commercial Applications:

- Enables system dessign and optimization of nanopore sequencers, Nanosensor arrays, Ion Channel Platforms etc..
- This effort will leverage work at CFDRC (Plasma, hybridization), and will generalize the approach for bio-applications.

EXTRA IMAGES


Time Scale
hours
seconds
microseconds
nanoseconds
picoseconds
Device Level:
• Convective-Diffusive Transport
• Surface/Volume Chemistry
Nanoscale:
• Molecular Dynamics
• Monte Carlo
• Quantum Mechanics
This Effort bridges the gap between Nanoscale and Device scale using methods such as Master Equation and Boltzmann's Equation to take molecular level information and use it in device level simulations.
1 nm
100 nm
1 μm
1 mm
1 m
Length Scale


minutes
seconds
microseconds
nanoseconds
picoseconds
Probability Distribution Function
Device Design
Continuum Modeling
Design Rules
Master Equation/ FPE
Molecular Level Modeling
Transition Rate Matrix
1 nm
100 nm
1 μm
1 mm
10 cm

COUPLING TO CONTINUUM SOLVER: RESULTS